

08/450437

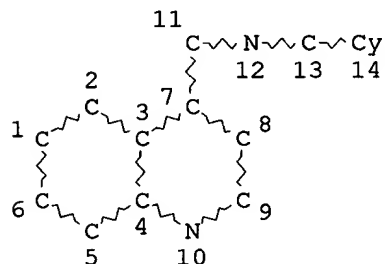
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=> fil reg; d que stat; fil ca,caplus; s 15 or 15/d
FILE 'REGISTRY' ENTERED AT 11:13:41 ON 17 JUN 1997
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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STRUCTURE FILE UPDATES: 15 JUNE 97 HIGHEST RN 189933-40-2
DICTIONARY FILE UPDATES: 16 JUNE 97 HIGHEST RN 189933-39-9
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TSCA INFORMATION NOW CURRENT THROUGH DECEMBER 1996

Please note that search-term pricing does apply when conducting SmartSELECT searches.

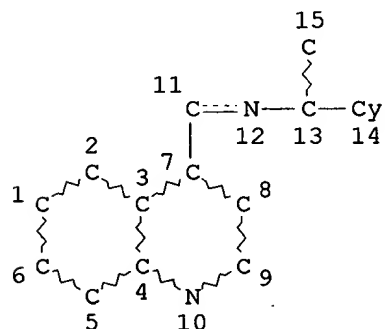
L1	STR
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NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RSPEC I  
NUMBER OF NODES IS 14

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STEREO ATTRIBUTES: NONE
L2          194 SEA FILE=REGISTRY SSS FUL L1
L4          STR
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NODE ATTRIBUTES:
NSPEC      IS RC      AT 15
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

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GRAPH ATTRIBUTES:  
RSPEC I

Searcher : Shears 308-4994

08/450437

NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE

L5 120 SEA FILE=REGISTRY SUB=L2 SSS FUL L4

100.0% PROCESSED 192 ITERATIONS

120 ANSWERS

SEARCH TIME: 00.00.03

FILE 'CA' ENTERED AT 11:13:42 ON 17 JUN 1997

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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FILE 'CAPLUS' ENTERED AT 11:13:42 ON 17 JUN 1997

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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L6 10 FILE CA

L7 11 FILE CAPLUS

TOTAL FOR ALL FILES

L8 21 L5 OR L5/D

=> dup rem l8; d 1-11 .bevstr; sel hit l7 1-11 rn

PROCESSING COMPLETED FOR L8

L9 11 DUP REM L8 (10 DUPLICATES REMOVED)

L9 ANSWER 1 OF 11 CAPLUS COPYRIGHT 1997 ACS

AN 1997:320920 CAPLUS

TI Discovery of a Novel Class of Selective Non-Peptide Antagonists for the Human Neurokinin-3 Receptor. 1. Identification of the 4-Quinolinecarboxamide Framework

AU Giardina, Giuseppe A. M.; Sarau, Henry M.; Farina, Carlo; Medhurst, Andrew D.; Grugni, Mario; Raveglia, Luca F.; Schmidt, Dulcie B.; Rigolio, Roberto; Luttmann, Mark; Vecchiotti, Vittorio; Hay, Douglas W. P.

CS Department of Chemistry, SmithKline Beecham S.p.A., Baranzate, 20021, Italy

SO J. Med. Chem. (1997), 40(12), 1794-1807  
CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

AB A novel class of potent and selective non-peptide neurokinin-3 (NK-3) receptor antagonists, featuring the 4-quinolinecarboxamide framework, was designed based upon chem. diverse NK-1 receptor antagonists. The novel compds., prompted by chem. modifications of the prototype, were characterized by binding anal. using a membrane prepn. of chinese hamster ovary (CHO) cells expressing the human neurokinin-3 receptors (hNK-3-CHO), and clear structure-activity relationships (SARs) were established. From SARs, (R)-N-[.alpha.-(methoxycarbonyl)benzyl]-2-phenylquinoline-4-carboxamide (I, SB 218795, hNK-3-CHO binding  $K_i$  = 13 nM) emerged as one of the most potent compds. of this novel class. Selectivity studies vs. the other neurokinin receptors (hNK-2-CHO and hNK-1-CHO)  
Searcher : Shears 308-4994

revealed that 65 is about 90-fold selective for hNK-3 vs. hNK-2 receptors (hNK-2-CHO binding  $K_i$  = 1221 nM) and over 7000-fold selective vs. hNK-1 receptors (hNK-1-CHO binding  $K_i$  = >100 .mu.M). In vitro functional studies in rabbit isolated iris sphincter muscle prepn. demonstrated that I a competitive antagonist of the contractile response induced by the potent and selective NK-3 receptor agonist senktide with a  $K_b$  = 43 nM. Overall, the data indicate that I is a potent and selective hNK-3 receptor antagonist and a useful lead for further chem. optimization.

IT RN LIST MAY NOT BE COMPLETE: 67-64-1 70-11-1 75-05-8 83-93-2  
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 189816-06-6

L9 ANSWER 2 OF 11 CA COPYRIGHT 1997 ACS DUPLICATE 1  
 AN 126:89156 CA ✓  
 TI Preparation of chiral isothiocyanates as derivatizing agents  
 IN Lindner, Wolfgang; Kleidernigg, Oliver Paul  
 PA Lindner, Wolfgang, Austria; Kleidernigg, Oliver Paul  
 SO PCT Int. Appl., 42 pp.  
 CODEN: PIXXD2  
 PI WO 9637465 A1 961128  
 DS W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE,  
 ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT,  
 LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE,  
 SG, SI  
 RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB,  
 GR, IE, IT, LU, MC, NL, PT, SE  
 AI WO 96-EP2258 960524  
 PRAI EP 95-108125 950526  
 DT Patent  
 LA English  
 OS MARPAT 126:89156  
 AB R1NHCHR2CHR3NCS [R1 = COR4, CO2R5, SO2R6; R2,R3 = aliph. or arom.  
 group; R2R3 = atoms to complete carbocyclic or heterocyclic ring; R4  
 Searcher : Shears 308-4994

= aliph. or (hetero)arom. group, aralkyl; R5 = CMe3, (nitro)benzyl, fluorenylmethyl; R6 = (hetero)aryl] were prepd. Thus, (R,R)-1,2-diaminocyclohexane was cyclocondensed with CS2 and the product amidated by 3,5-(O2N)2C6H3COCl to give (R,R)-N-(2-isothiocyanatocyclohexyl)-3,5-dinitrobenzamide. The latter was used to prep. diastereomeric derivs. of (R)-, and (S)-propranolol. Data for chromatog. sepns. of, e.g., amino acids, etc. were given.

IT **185508-91-2P 185508-92-3P**

RL: NUU (Nonbiological use, unclassified); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)  
(prepn. of chiral isothiocyanates as derivatizing agents)

L9 ANSWER 3 OF 11 CA COPYRIGHT 1997 ACS DUPLICATE 2  
AN 125:25636 CA

TI 2-Phenyl-4-quinolinecarboxamides: A Novel Class of Potent and Selective Non-Peptide Competitive Antagonists for the Human Neurokinin-3 Receptor

AU Giardina, Giuseppe A. M.; Sarau, Henry M.; Farina, Carlo; Medhurst, Andrew D.; Grugni, Mario; Foley, James J.; Raveglia, Luca F.; Schmidt, Dulcie B.; Rigolio, Roberto; et al.

CS Department of Chemistry, SmithKline Beecham S.p.A., Baranzate, 20021, Italy

SO J. Med. Chem. (1996), 39(12), 2281-2284  
CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

OS CJACS-IMAGE; CJACS

AB A novel class of potent and selective, non-peptide NK-3 receptor antagonists, based on the 2-phenylquinoline framework, has been identified and characterized by binding anal. using membrane prepn. of CHO cells expressing the human neurokinin receptors (hNKs-CHO). Functional activity was detd. by inhibition of senktide-induced contraction of the rabbit isolated iris sphincter muscle prepn. An extensive structure-activity study led to the identification of (S)-(-)-N-(.alpha.-ethylbenzyl)-3-hydroxy-2-phenylquinoline-4-carboxamide (SB 223412) as the most potent ( $K_i = 1.0$  nM in hNK-3-CHO binding;  $K_b = 5.4$  nM for antagonism of senktide-induced contraction in rabbit iris sphincter muscle) and selective (hNK-2/hNK-3  $K_i$  ratio of 144 and hNK-1/hNK-3  $K_i$  ratio  $> 100,000$ ) hNK-3 receptor antagonist of this class. In addn., NKB-induced  $Ca^{2+}$  mobilization studies in hNK-3-HEK 293 cells indicated that SB 223412 is a reversible, competitive antagonist. Compds. from this novel class will be extremely useful in the functional characterization of hNK-3 receptors and elucidation of potential therapeutic indications for selective hNK-3 receptor antagonists.

IT **174635-51-9P 174635-52-0P 174635-53-1P**  
**174635-69-9P 174636-20-5P 174636-32-9P,**  
SB 223412

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
(prepn. and structure-activity of human neurokinin 3 receptor antagonists phenylquinolinecarboxamides)

L9 ANSWER 4 OF 11 CA COPYRIGHT 1997 ACS DUPLICATE 3  
AN 124:232269 CA

TI Quinoline derivatives as tachykinin NK3 receptor antagonists

IN Farina, Carlo; Giardina, Giuseppe Arnaldo Mari; Grugni, Mario; Raveglia, Luca Francesco

PA Smithkline Beecham Farmaceutici S.P.A., Italy

SO PCT Int. Appl., 95 pp.

08/450437

CODEN: PIXXD2

PI WO 9532948 A1 951207

DS W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI,  
GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD,  
MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ,  
TM, TT

RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR,  
IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG

AI WO 95-EP2000 950523

PRAI IT 94-MI1099 940527

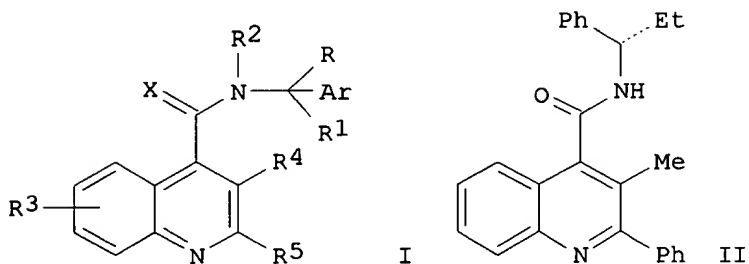
IT 95-MI494 950314

DT Patent

LA English

OS MARPAT 124:232269

GI



AB NK3 receptor antagonists I (Ar = (un)substituted Ph, naphthyl, cycloalkadienyl, heteroaryl; R = (un)substituted alkyl, cycloalkyl, (un)substituted Ph, phenylalkyl, or heteroaryl, CO<sub>2</sub>H and derivs., etc.; R<sup>1</sup>, R<sup>2</sup> = H, alkyl; or R<sup>1</sup>R<sup>2</sup> = (CH<sub>2</sub>)<sub>3-5</sub>; or RR<sup>1</sup> = (CH<sub>2</sub>)<sub>2-5</sub>; R<sup>3</sup>, R<sup>4</sup> = H, alkyl, alkenyl, aryl, alkoxy, OH, halo, NO<sub>2</sub>, amino, etc.; R<sup>5</sup> = alkyl, cycloalkyl, (un)substituted (hetero)aryl; X = O, S, N(CN)] are useful in treating pulmonary, CNS, and neurodegenerative disorders, etc. Approx. 115 compds. were prepd. For example, amidation of 3-methyl-2-phenylquinoline-4-carbonyl chloride with (R)-.alpha.-ethylbenzylamine gave title compd. II in 58% yield. II had IC<sub>50</sub> of 5.6 nM for displacement of [3H]-senktide from guinea-pig cortical NK3 receptors. Antagonist activity of I was shown by inhibition of senktide-induced contraction of guinea-pig ileum.

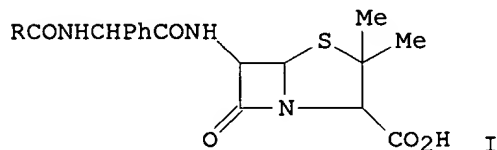
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174635-91-7P 174635-92-8P 174635-93-9P  
174635-94-0P 174635-95-1P 174635-96-2P

Searcher : Shears 308-4994

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RL: BAC (Biological activity or effector, except adverse); SPN  
 (Synthetic preparation); THU (Therapeutic use); BIOL (Biological  
 study); PREP (Preparation); USES (Uses)  
 (prepn. of quinolinecarboxamide derivs. as tachykinin NK3  
 receptor antagonists)

L9 ANSWER 5 OF 11 CA COPYRIGHT 1997 ACS DUPLICATE 4  
 AN 93:186338 CA  
 TI Ampicillin derivatives  
 PA Mitsubishi Yuka Yakuhin Co., Ltd., Japan  
 SO Jpn. Kokai Tokkyo Koho, 10 pp.  
 CODEN: JKXXAF  
 PI JP 55055194 800422 Showa  
 AI JP 78-127324 781018  
 DT Patent  
 LA Japanese  
 GI



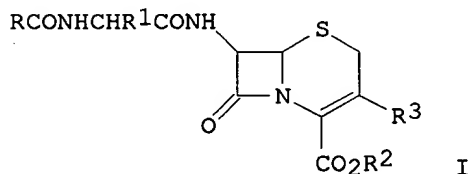
AB Fifteen title derivs. I (R = heterocyclic, heterocyclic-substituted  
 methyl) were prepd. and the min. inhibition concns. treated against  
 Ps. aeruginosa, St. aureus, B. subtilis, E. coli, Kl. pneumoniae,  
 and Pr. vulgaris. Thus, 618 mg DCC was added to a mixt. of 648  
 4-carbamoyl-2-quinolinecarboxylic acid and 345 mg  
 N-hydroxysuccinimide in DMF with ice cooling, the mixt. stirred 10 h  
 with ice cooling, a mixt. of 1.2 g ampicillin-3H<sub>2</sub>O and 0.42 mL Et<sub>3</sub>N  
 in CH<sub>2</sub>Cl<sub>2</sub>-DMF added, and the mixt. stirred 3 h at room temp. to  
 give, after treating with K 2-ethylhexanoate, 1.32 d-I (R =  
 4-carbamoyl-2-quinolyl) K salt.  
 IT 75204-90-9P

Searcher : Shears 308-4994

08/450437

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (prepn. and bactericidal activity of)

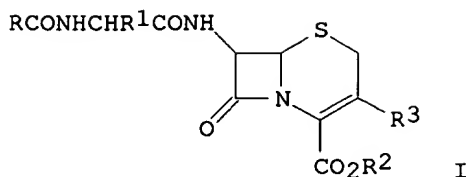
L9 ANSWER 6 OF 11 CA COPYRIGHT 1997 ACS DUPLICATE 5  
AN 90:38949 CA  
TI Cephalosporins with .alpha.-acylaminoacetic acid side chains  
IN Kocsis, Karoly; Peter, Heinrich; Bickel, Hans  
PA Ciba-Geigy A.-G., Switz.  
SO Swiss, 11 pp.  
CODEN: SWXXAS  
PI CH 606006 781013  
AI CH 74-6494 740513  
DT Patent  
LA German  
GI



AB The cephalosporins I [R = 6-membered ring contg. 1-3 N atoms and an oxo group (optionally substituted or condensed with other rings); R<sup>1</sup> = (substituted) Ph, thienyl, furyl, cyclohexadienyl; R<sup>2</sup> = H, ester group; R<sup>3</sup> = H, alkoxy, substituted Me] were prepd. for use as bactericides, e.g., at 8-100 mg/kg s.c. in mice against Staphylococcus aureus. Thus, D-(-)-(1,6-dihydro-6-oxo-3-pyridazinylcarbonylamino)phenylacetic acid reacted with ClCO<sub>2</sub>Et, N-methylmorpholine, and 7.beta.-aminocephalosporanic acid in THF to give D-7.beta.-I (R = 1,6-dihydro-6-oxo-3-pyridazinyl, R<sup>1</sup> = Ph, R<sup>2</sup> = H, R<sup>3</sup> = AcOCH<sub>2</sub>).

IT **59133-55-0P**  
RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

L9 ANSWER 7 OF 11 CA COPYRIGHT 1997 ACS DUPLICATE 6  
AN 90:38951 CA  
TI Cephalosporins with .alpha.-acylaminoacetic acid side chains  
IN Kocsis, Karoly; Peter, Heinrich; Bickel, Hans  
PA Ciba-Geigy A.-G., Switz.  
SO Swiss, 11 pp.  
CODEN: SWXXAS  
PI CH 606001 781013  
AI CH 74-6494 740513  
DT Patent  
LA German  
GI



AB The cephemcarboxylic acids I [R = 6-membered ring contg. 1-3 N atoms and an oxo group, optionally substituted or condensed with other rings; R1 = (substituted) Ph, thienyl, furyl, cyclohexadienyl; R2 = H, physiolo. cleavable ester group; R3 = H, (substituted) Me, lower alkoxy] were prepd. for use as bactericides, e.g., at 8-100 mg/kg s.c. against *Staphylococcus aureus* in mice. Thus, cephaloglycin reacted with 6-hydroxy-3-pyridinecarbonyl chloride in CH<sub>2</sub>Cl<sub>2</sub> to give I (R = 6-hydroxy-3-pyridyl, R1 = Ph, R2 = H, R3 = CH<sub>2</sub>OAc).

IT **59133-55-0P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

L9 ANSWER 8 OF 11 CA COPYRIGHT 1997 ACS

DUPLICATE 7

AN 84:135637 CA

TI Penicillins

IN Tobiki, Hisao; Shimaji, Kozo; Okano, Shigeru; Komatsu, Toshiaki;

Katsura, Toyozo; Taira, Yasushi; Eda, Yasuko

PA Sumitomo Chemical Co., Ltd., Japan

SO Japan., 11 pp.

CODEN: JAXXAD

PI JP 50023036 B4 750805 Showa

AI JP 70-124363 701229

DT Patent

LA Japanese

GI For diagram(s), see printed CA Issue.

AB Acids ROH I (Z = O, S; R1 = alkyl, cycloalkylalkyl, alkenyl, aralkyl, OH, alkoxy, aralkyloxy; R2 = H, alkyl; A = benzo, naphtho, pyrido) were treated with 6-aminopenicillanic acid (III) or its derivs. to give II. II are bactericides not only against gram-pos. and -neg. bacteria but also against *Pseudomonas aeruginosa* (min. inhibitory concn. 3.13-50 .mu.g/ml). Thus, 2 g 1-hydroxy-6,7-methylenedioxy-4-quinolone-3-carboxylic acid in CH<sub>2</sub>Cl<sub>2</sub> was treated with Et<sub>3</sub>N, 1.8 g ClCO<sub>2</sub>Et, and 1.65 g D(-)-.alpha.-phenylglycine Et ester-HCl to give 1.8 g D(-)-.alpha.-(1-hydroxy-6,7-methylenedioxy-4-quinolone-3-carboxamido)phenylacetic acid, which (1 g) in CH<sub>2</sub>Cl<sub>2</sub> was treated with Et<sub>3</sub>N, ClCO<sub>2</sub>Et and 0.83 g III Et<sub>3</sub>N salt to give 1.3 g D(-)-II (Z = O, R1 = OH, R2 = H, A = 6,7-methylenedioxybenzo). Among 25 more II prepd. were (Z, R1, R2, A given): O, Et, H, 6-methoxybenzo; O, Me, H, X; O, Et, H, 1,2-naphtho; O, OEt, H, 6,7-methylenedioxybenzo.

IT **58865-82-0P**

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
(prepn. and bactericidal activity of)

L9 ANSWER 9 OF 11 CA COPYRIGHT 1997 ACS

DUPLICATE 8

AN 84:164802 CA

TI Cephalosporins with .alpha.-acylaminoacetic acid side chain

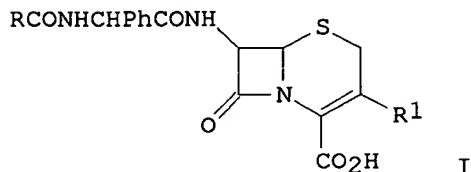
IN Kocsis, Karoly; Peter, Heinrich; Bickel, Hans

PA Ciba-Geigy A.-G., Switz.

Searcher : Shears 308-4994



SO Ger. Offen., 80 pp.  
 CODEN: GWXXBX  
 PI DE 2520561 751127  
 PRAI CH 74-6494 740513  
 DT Patent  
 LA German  
 GI



AB Of the cephalosporins I (R = N heterocyclyl, R1 = CH2OAc, OMe, heterocyclic thiomethyl pyridiniomethyl) were prepd. by acetylating cephaloglycines and substituting on acetoxymethyl group. Thus, I (R = 2-hydroxy-5-pyridyl, R1 = OAc) was obtained by treating cephaloglycine with 2-hydroxy-5-pyridinecarbonyl chloride.

IT **59133-55-0P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

L9 ANSWER 10 OF 11 CA COPYRIGHT 1997 ACS DUPLICATE 9

AN 70:47439 CA  
 TI .alpha.-Amidobenzyl- and amido(2-thienyl)methylpenicillins  
 IN Long, Anthony Alfred W.; Nayler, John H. C.  
 PA Beecham Group Ltd.  
 SO Brit., 6 pp.  
 CODEN: BRXXAA  
 PI GB 1130445 681016  
 AI GB 660426  
 DT Patent  
 LA English  
 GI For diagram(s), see printed CA Issue.

AB The 6-aminopenicillanic acid derivs. prepd. had the structure I, where R is a Ph or thienyl group, R1 is a heterocyclic group, and n is 0 or 1. The compds. were useful as antibacterial agents, as nutritional supplements in animal food, and in the treatment of infectious diseases caused by gram-pos. and gram-neg. bacteria. Thus, a suspension of 12.8 g. D-.alpha.-aminobenzylpenicillin (II) trihydrate in 80 ml. H2O was adjusted to pH 9.2 with 5N aq. NaOH and treated with a soln. of 4.6 g. 5-methyl-3-isoxazolecarbonyl chloride in 100 ml. iso-BuCOMe (III). After stirring for 2 hrs. at room temp., the mixt. was filtered through Dicalite and the layers were sepd. The org. phase was washed with satd. brine and treated with 16 ml. 2N Na 2-ethylhexanoate in III to give 13 g. Na salt of D-.alpha.-(5-methyl-3-iso-xazolecarboxamido)benzylpenicillin which crystd. on trituration with ether. The sodium salts of D-.alpha.-(5-methyl-4-isoxazolecar-boxamido)benzylpenicillin, D-.alpha.-(2-furancarboxamido)benzylpenicillin, D-.alpha.-(3-thiophenecarboxamido)benzylpenicillin, D-.alpha.-(2-thiophenecarboxamido)benzylpenicillin, D-.alpha.-(2-thiopheneacetamido)benzylpenicillin, D-.alpha.-(3-thiopheneacetamido)benzylpenicillin, D-.alpha.-(3-ethoxy-4-quinolinecarboxamido)benzylpenicillin, D-.alpha.-(8-methoxy-2-

Searcher : Shears 308-4994

quinolinecarboxamido)benzylpenicillin, D-.alpha.-(2-pyridinecarboxamido)benzylpenicillin, D-.alpha.-(phthalimidoacetamido)-benzylpenicillin, D-.alpha.-(2,6-dioxo-4-piperidineacetamido)benzylpenicillin, D-.alpha.-(2-oxo-2H-pyran-5-carboxamido)benzylpenicillin, D-.alpha.-(5-methyl-3-phenyl-4-isoxazolecarboxamido)benzylpenicillin, D-.alpha.-(3-methyl-5-phenyl-4-isoxazolecarboxamido)benzylpenicillin, D-.alpha.-(5-bromo-2-(methylthio)-4-pyrimidinecarboxamido)benzylpenicillin, D-.alpha.-(2-furoylamino)-2-thienylmethylpenicillin, D-.alpha.-nicotinamidobenzylpenicillin, D-.alpha.-(2-thiopheneacetamido)-2-thi-enylmethylpenicillin, and D-.alpha.-(2-furanacetamido)benzylpenicillin were similarly prepd.

IT **21611-82-5P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

L9 ANSWER 11 OF 11 CA COPYRIGHT 1997 ACS DUPLICATE 10  
AN 74:87972 CA  
TI Antibacterial acylated benzylpenicillin and thienylmethylpenicillin derivatives  
PA Beecham Group Ltd.  
SO Fr. M., 4 pp.  
CODEN: FMXXAJ  
PI FR 6212 680902  
PRAI GB 660426  
DT Patent  
LA French  
GI For diagram(s), see printed CA Issue.  
AB [.alpha.-(Amino)arylacetamido]penicillin deriv. (I), where Ar is Ph or 2-thienyl, are treated with Ar1(CH2)nCOCl (Ar1 = heteroaryl) to give penicillin diamide derivs. (II). II (n = 0 or 1 and Ar1 is furyl, thienyl, phthalimido, or a substituted quinolyl, piperidyl, oxopyranyl, or isoxazolyl group) are prepd.  
IT **21611-82-5P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

E1 THROUGH E120 ASSIGNED

=> fil reg

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DICTIONARY FILE UPDATES: 16 JUNE 97 HIGHEST RN 189933-39-9

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Searcher : Shears 308-4994

08/450437

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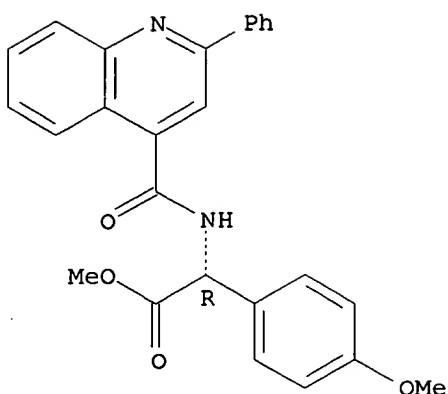
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L10 ANSWER 1 OF 120 REGISTRY COPYRIGHT 1997 ACS  
RN **189815-94-9** REGISTRY  
CN INDEX NAME NOT YET ASSIGNED  
FS 3D CONCORD; STEREOSEARCH  
MF C26 H22 N2 O4  
SR CA  
LC STN Files: CAPLUS

PS

Absolute stereochemistry.

08/450437

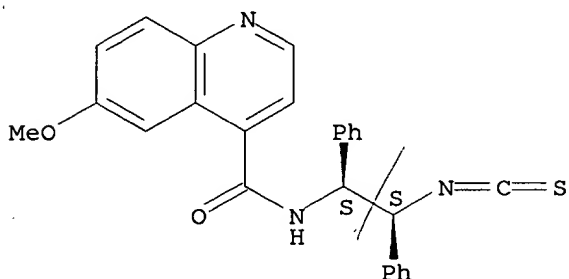


1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L10 ANSWER 4 OF 120 REGISTRY COPYRIGHT 1997 ACS  
RN **185508-92-3** REGISTRY  
CN 4-Quinolinecarboxamide, N-(2-isothiocyanato-1,2-diphenylethyl)-6-methoxy-, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD; STEREOSEARCH  
MF C26 H21 N3 O2 S  
SR CA  
LC STN Files: CA, CAPLUS

L9 2 only

Absolute stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)

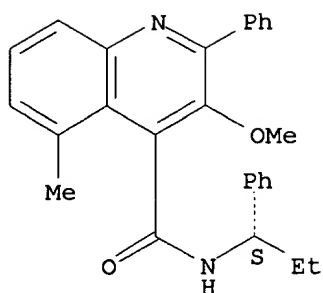
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L10 ANSWER 6 OF 120 REGISTRY COPYRIGHT 1997 ACS  
RN **174636-62-5** REGISTRY  
CN 4-Quinolinecarboxamide, 3-methoxy-5-methyl-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C27 H26 N2 O2  
SR CA  
LC STN Files: CA, CAPLUS

2 hts  
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Absolute stereochemistry.

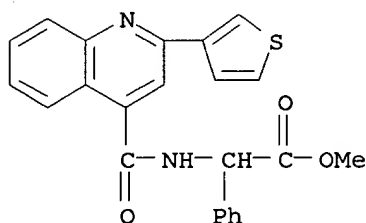
08/450437



1 REFERENCES IN FILE CA (1967 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L10 ANSWER 67 OF 120 REGISTRY COPYRIGHT 1997 ACS  
RN **174635-98-4** REGISTRY  
CN Benzeneacetic acid, .alpha.-[[[2-(3-thienyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C23 H18 N2 O3 S  
SR CA  
LC STN Files: CA, CAPLUS

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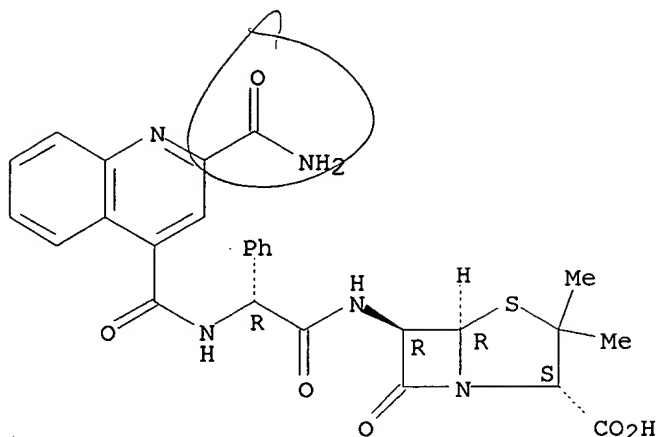


1 REFERENCES IN FILE CA (1967 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L10 ANSWER 117 OF 120 REGISTRY COPYRIGHT 1997 ACS  
RN **75204-90-9** REGISTRY  
CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[[[2-(aminocarbonyl)-4-quinolinyl]carbonyl]amino]phenylacetyl]amino]-3,3-dimethyl-7-oxo-, monopotassium salt, [2S-[2.alpha.,5.alpha.,6.beta.(S\*)]]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C27 H25 N5 O6 S . K  
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

08/450437

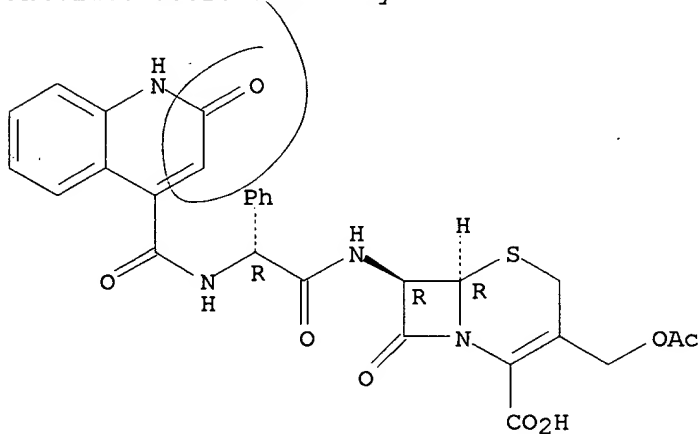


● K

1 REFERENCES IN FILE CA (1967 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L10 ANSWER 118 OF 120 REGISTRY COPYRIGHT 1997 ACS  
RN **59133-55-0** REGISTRY  
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
3-[(acetyloxy)methyl]-7-[[[(1,2-dihydro-2-oxo-4-  
quinolinyl)carbonyl]amino]phenylacetyl]amino]-8-oxo-,  
[6R-[6.alpha.,7.beta.(R\*)]]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C28 H24 N4 O8.S  
LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

Absolute stereochemistry.



3 REFERENCES IN FILE CA (1967 TO DATE)  
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

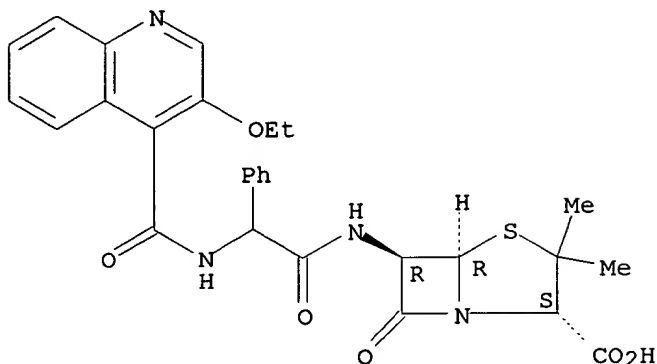
L10 ANSWER 119 OF 120 REGISTRY COPYRIGHT 1997 ACS  
RN **58865-82-0** REGISTRY  
CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid,  
6-[[[(3-ethoxy-4-quinolinyl)carbonyl]amino]phenylacetyl]amino]-3,3-  
dimethyl-7-oxo-, monosodium salt, [2S-(2.alpha.,5.alpha.,6.beta.)]-  
Searcher : Shears 308-4994

/L.t. *See new L/8*

08/450437

(9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C28 H28 N4 O6 S . Na  
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

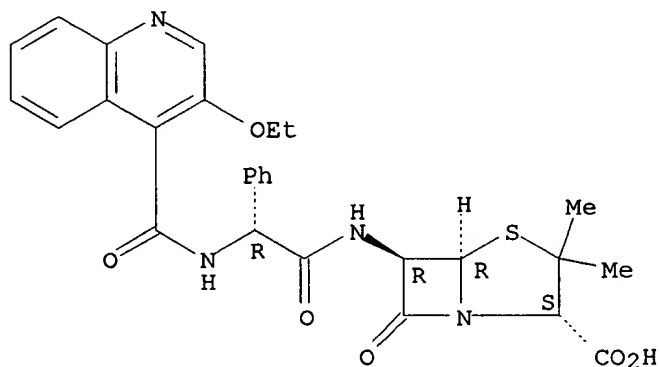


● Na

1 REFERENCES IN FILE CA (1967 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L10 ANSWER 120 OF 120 REGISTRY COPYRIGHT 1997 ACS  
RN **21611-82-5** REGISTRY  
CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid,  
6-[2-(3-ethoxycinchoninamido)-2-phenylacetamido]-3,3-dimethyl-7-oxo-  
, D- (8CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C28 H28 N4 O6 S  
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



*2 h. B see new Lm  
pushy optically subst  
5 methyl ketone*

2 REFERENCES IN FILE CA (1967 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

08/450437

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FILE LAST UPDATED: 30 OCT 91 (910803/ED)

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substance identification.

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format. See NEWS for details.

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L11 0 L10

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CA INDEXING COPYRIGHT (C) 1997 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 10 Jun 1997 (19970610/PD)  
FILE LAST UPDATED: 11 Jun 1997 (970611/ED)  
HIGHEST PATENT NUMBER: US5638543  
CA INDEXING IS CURRENT THROUGH 11 Jun 1997 (970611/UPCA)  
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 10 Jun 1997 (19970610/PD)  
REVISED CLASS FIELDS (/NCL) CURRENT THROUGH: APR 1997  
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: FEB 1997

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>>> available for the WIPO International Patent Classification <<<  
>>> (IPC) Manuals, editions 1-6, in the /IC1, /IC2, /IC3, /IC4, <<<  
>>> /IC5, and /IC (/IC6) fields, respectively. The thesauri in <<<  
>>> the /IC5 and /IC fields include the corresponding catchword <<<  
>>> terms from the IPC subject headings and subheadings. <<<

This file contains CAS Registry Numbers for easy and accurate  
substance identification.

L12 3 L10

=> d 1-3 bib abs hitstr; fil marpat

L12 ANSWER 1 OF 3 USPATFULL  
AN 81:24739 USPATFULL  
TI Cephalosporins having an .alpha.-acylaminoacetic acid side chain  
IN Kocsis, Karoly, Basel, Switzerland  
Peter, Heinrich, Binningen, Switzerland  
Bickel, Hans, Binningen, Switzerland  
PA Ciba-Geigy Corporation, Ardsley, NY, United States (U.S.)  
Searcher : Shears 308-4994



08/450437

corporation)  
PI US 4265892 810505  
AI US 79-11359 790212 (6)  
RLI Division of Ser. No. US 77-789164, filed on 20 Apr 1977, now  
patented, Pat. No. US 4154831 which is a division of Ser. No. US  
75-576398, filed on 9 May 1975, now patented, Pat. No. US 4041161  
PRAI CH 74-6494 740513  
DT Utility  
EXNAM Primary Examiner: Coughlan, Jr., Paul M.  
LREP Almaula, Prabodh I.  
CLMN Number of Claims: 10  
ECL Exemplary Claim: 1,7  
DRWN No Drawings  
LN.CNT 1140

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Compounds of the formula ##STR1## wherein R.sub.1 denotes  
optionally substituted phenyl, thienyl, furyl or  
1,4-cyclohexadienyl, R.sub.2 represents a free carboxyl group or  
an esterified carboxyl group which can be split physiologically,  
R.sub.3 represents hydrogen, lower alkoxy or an optionally  
substituted methyl group and B represents an optionally substituted  
six-membered ring with 1 to 3 ring nitrogen atoms, which is bonded  
to the carbonyl group --C(.dbd.O)-- by one of its carbon atoms,  
the nitrogen atoms of a monocyclic six-membered ring having 2  
nitrogen atoms being either adjacent or separated by two ring  
carbon atoms, and the salts of such compounds which have a  
salt-forming group, including the inner salts, for example the  
7.beta.-[D(-)-.alpha.-(3,5-Dioxo-2,3,4,5-tetrahydro-1,2,4-triazine-  
6-carboxamido)-phenylacetamido]-cephalosporanic acid, have  
antibiotic activity.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

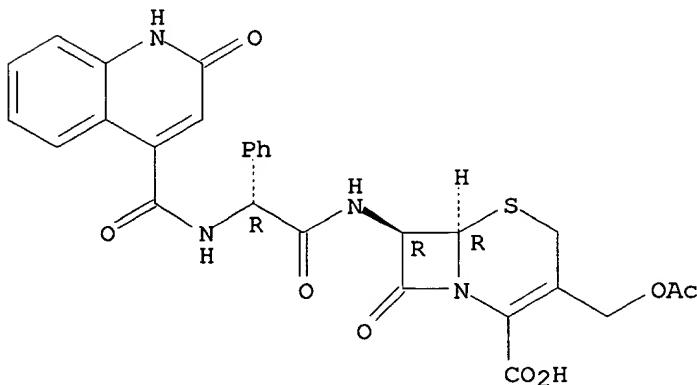
IT 59133-55-0P

(prepn. of)

RN 59133-55-0 USPATFULL

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
3-[(acetyloxy)methyl]-7-[[[(1,2-dihydro-2-oxo-4-  
quinolinyl)carbonyl]amino]phenylacetyl]amino]-8-oxo-,  
[6R-[6.alpha.,7.beta.(R\*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



08/450437

AN 79:24260 USPATFULL  
TI Cephalosporins having an .alpha.-acylaminoacetic acid side chain  
IN Kocsis, Karoly, Basel, Switzerland  
Peter, Heinrich, Binningen, Switzerland  
Bickel, Hans, Binningen, Switzerland  
PA Ciba-Geigy Corporation, Ardsley, NY, United States (U.S.  
corporation)  
PI US 4154831 790515  
AI US 77-789164 770420 (5)  
RLI Division of Ser. No. US 75-576398, filed on 9 May 1975, now  
patented, Pat. No. US 4041161  
PRAI CH 74-6494 740513  
DT Utility  
EXNAM Primary Examiner: Daus, Donald G.; Assistant Examiner: Wheeler,  
David E.  
LREP Maitner, John J.  
CLMN Number of Claims: 8  
ECL Exemplary Claim: 1,4  
DRWN No Drawings  
LN.CNT 1119  
CAS INDEXING IS AVAILABLE FOR THIS PATENT.  
AB Compounds of the formula ##STR1## wherein R.sub.1 denotes  
optionally substituted phenyl, thienyl, furyl or  
1,4-cyclohexadienyl, R.sub.2 represents a free carboxyl group or  
an esterified carboxyl group which can be split physiologically,  
R.sub.3 represents hydrogen, lower alkoxy or an optionally  
substituted methyl group and B represents an optionally  
substituted six-membered ring with 1 to 3 ring nitrogen atoms,  
which is bonded to the carbonyl group --C(.dbd.O)-- by one of its  
carbon atoms, the nitrogen atoms of a monocyclic six-membered ring  
having 2 nitrogen atoms being either adjacent or separated by two  
ring carbon atoms, and the salts of such compounds which have a  
salt-forming group, including the inner salts, for example the  
7.beta.-[D(-)-.alpha.-(3,5-Dioxo-2,3,4,5-tetrahydro-1,2,4-triazine-  
6-carboxamido)-phenylacetamido]-cephalosporanic acid, have  
antibiotic activity.

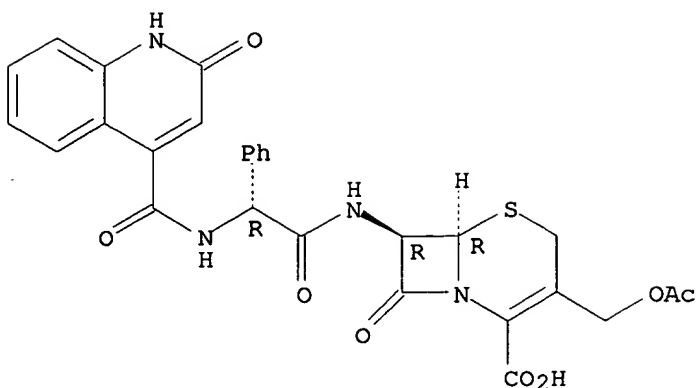
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT **59133-55-0P**  
(prepn. of)

RN 59133-55-0 USPATFULL

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
3-[(acetyloxy)methyl]-7-[[[(1,2-dihydro-2-oxo-4-  
quinolinyl)carbonyl]amino]phenylacetyl]amino]-8-oxo-,  
[6R-[6.alpha.,7.beta.(R\*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 3 OF 3 USPATFULL

AN 77:41963 USPATFULL

TI Cephalosporins having an .alpha.-acylaminoacetic acid side chain

IN Kocsis, Karoly, Basel, Switzerland

Peter, Heinrich, Binningen, Switzerland

Bickel, Hans, Binningen, Switzerland

PA Ciba-Geigy Corporation, Ardsley, NY, United States (U.S. corporation)

PI US 4041161 770809

AI US 75-576398 750509 (5)

PRAI CH 74-6494 740513

DT Utility

EXNAM Primary Examiner: Rizzo, Nicholas S.; Assistant Examiner: Wheeler, David E.

LREP Kolodny, Joseph G.; Maitner, John J.; Groeger, Theodore O.

CLMN Number of Claims: 6

ECL Exemplary Claim: 1,5

DRWN No Drawings

LN.CNT 1095

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Compounds of the formula ##STR1## wherein R.sub.1 denotes optionally substituted phenyl, thienyl, furyl or 1,4-cyclohexadienyl, R.sub.2 represents a free carboxyl group or an esterified carboxyl group which can be split physiologically, R.sub.3 represents hydrogen, lower alkoxy or an optionally substituted methyl group and B represents an optionally substituted six-membered ring with 1 to 3 ring nitrogen atoms, which is bonded to the carbonyl group --C(=O)-- by one of its carbon atoms, the nitrogen atoms of a monocyclic six-membered ring having 2 nitrogen atoms being either adjacent or separated by two ring carbon atoms, and the salts of such compounds which have a salt-forming group, including the inner salts, for example the 7.beta.-[D(-)-.alpha.-(3,5-Dioxo-2,3,4,5-tetrahydro-1,2,4-triazine-6-carboxamido)-phenylacetamido]-cephalosporanic acid, have antibiotic activity.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 59133-55-0P

(prepn. of)

RN 59133-55-0 USPATFULL

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

3-[(acetyloxy)methyl]-7-[[[(1,2-dihydro-2-oxo-4-

Searcher : Shears 308-4994